



An experimentally-validated multi-scale materials, process and device modelling & design platform enabling non-expert access to open innovation in the Organic and Large Area Electronics Industry (MUSICODE)

Grand Agreement: 953187

Project Start Date: 01/01/2021

Project Duration: 48 months

Deliverable 2.7

Continuum modelling of solution processing by continuum mechanics

Date: 30-06-2023



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"

Project co-funded by the European Commission within Horizon 2020 Research and Innovation Programme		
Dissemination Level		
PU	Public	
PP	Restricted to other programme participants (including the Commission Service)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (excluding the Commission Services)	x

Deliverable author(s): Dr.-Ing. Aron Kneer, Dipl.-Ing. Klaus Reimann

Contributors: TinniT, AUTH, OET, UoI

Draft Revisions: v1.2 submitted to coordinator 22/06/2023
v2.0 approved by coordinator 26/06/2023

Copyright

@ Copyright 2021-2024 The MUSICODE Consortium

Consisting of Coordinator:	University of Ioannina (UoI)	Greece
Partners:	Karlsruhe Institute of Technology (KIT)	Germany
	University of Surrey (SURREY)	UK
	Aristotle University of Thessaloniki (AUTH)	Greece
	Czech Technical University in Prague (CVUT)	Czechia
	Fluxim AG (FLUXIM)	Switzerland
	TinniT Technologies GmbH (TINNIT)	Germany
	Granta design LTD (GRANTA)	UK
	Esteco SPA (ESTECO)	Italy
	Organic Electronic Technologies (OET)	Greece
	Apeva SE (APEVA)	Germany
	ANSYS (ANSYS)	UK
	AIXTRON SE (AIXTRON)	Germany

This document may not be copied, reproduced, or modified in whole or in part for any purpose without written permission from the MUSICODE Consortium. In addition to such written permission to copy, reproduce, or modify this document in whole or part, an acknowledgment of the authors of the document and all applicable portions of the copyright notice must be clearly referenced.

All Rights reserved.



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call

DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"

"The European Commission support for the production of this publication does not constitute an endorsement of the contents which reflects the views only of the authors, and the Commission cannot be held responsible for any use which may be made of the information contained therein."

Contents

Publishable summary	4
1. Introduction	5
1.1 Objectives of WP/Task.....	5
1.1 Purpose of this Document.....	6
2. Methodology	7
2.1 Some CFD basics and short description of the TinFlow solver	7
2.2 Theory of the film-model.....	7
2.2.1 Temperature-dependent Evaporation	8
2.2.2 Evaluation of the film model	8
2.3 Fluid property database of TinFlow.....	10
2.3.1 Embedded polynomials for property calculation	10
2.3.2 Datasheet structure.....	11
2.3.3 Properties of Toluene, o-Xylene and Air	12
2.4 Model set-up and results from reference case	14
2.4.1 Slot-die.....	14
2.4.2 Dryer	17
2.4.3 Dryer Reference Case Setup.....	18
2.4.4 Dryer Results of Reference Case	19
3. Results of dryer simulation studies	22
4. Experiments planned	26
5. Discussion	26
5.1 Achievements	26
5.2 Risks	26
5.2 Next steps	26
6. Conclusions	26
References	27

Publishable summary

For the production of organic photovoltaic cells, the cost-effective wet process is used for mass production. In this process conjugated polymers and functionalized molecules are applied to a substrate together with a solvent as a liquid phase. The liquid layer is applied using an application system known as slot-die. The essential component of this system is a flat nozzle, which has approximately the width of the substrate and a defined distance from the substrate. The flow behavior of the dispersion can be influenced by optional heating in the slot die (hot end). The layer thickness of the liquid can be controlled by the applied mass flow, the nozzle spacing and the rotational speed of the cylinder in the R2R process or the belt speed in a flat system.

The formation of a defined structure from the liquid film takes place in a conditioning chamber. A key feature of this conditioning chamber is the heating of the substrate, which leads to a slowly evaporation of the solvent. Air or nitrogen flows through the conditioning chamber are used to remove the evaporated solvent. Due to the evaporation of the solvent, the polymers separate, and a bi-continuous structure is created, which thickness has only a fraction of the thickness of the original liquid film.

Computational fluid dynamics (CFD) is an established method to compute in a two or three-dimensional domain the flow field. The numerical solution of the Navier-Stokes equations is based on the discretization of the conservation equations. A common discretization scheme is the finite volume method. The simulation domain is therefore discretized by finite volumes. The discretized conservation equations are partial differential equations which are nonlinear. Fluid mechanics is a subfield of continuum mechanics.

To be able to predict the above-mentioned production process different physics have to be addressed. First, predicting the wet coating process the volume of fluid approach is needed which enables the simulation of a phase interface between gas and liquid and represents therefore a 2-phase simulation method. For the drying process in the conditioning chamber a film-model has been developed which interacts with the gas flow which is being numerically solved using the discretized Navier-Stokes-equation. To solve for the thermodynamic mixing (thermal and gas components) process the energy and concentration equations with the integrated gas-law is needed. The film model itself delivers the evaporation rate and film thickness. The evaporated solvent is added as mass source to the gas flow. Phase separation is solved using the phase field approach of the partner KIT in another scale (μm) using the film conditions from the macro scale (m).

For the MUSICODE modelling platform for the coating and drying process enhanced CFD-models have been developed and tested within WP2. Realistic model dimensions and operation conditions specified by OET and AUTH have been used to set up two separate models addressing the slot-die and the dryer. To be able to use the results of the slot-die model it has been directly linked to the dryer model transferring the resulting film thickness and film conditions (temperature, concentration). Further scales to be addressed via transferring data, are from the dryer to the phase separation model (KIT) and from that scale to the molecular dynamics model (UoI) is to be addressed in the cross-scale workflow of the modeling platform.